

# **Michael E. Wall**

## **CURRICULUM VITAE**

(Updated 2/4/10)

### **Personal Data**

Citizenship: USA

Work Address: Mail Stop B256  
Information Sciences Group  
Computer, Computational, and Statistical Sciences Division  
Los Alamos National Laboratory  
Los Alamos, NM 87545

**Position** Scientist

**Education** B.S. Physics, University of California, San Diego (1989)  
Ph.D. Physics, Princeton University (1996), Thesis advisor: Sol Gruner

### **Professional Appointments**

1996-1999	Postdoctoral Fellow, Dept of Biochemistry and Cell Biology and Keck Center for Computational Biology, Rice University. Postdoctoral advisor: George N. Phillips, Jr.
1999-2001	Postdoctoral Research Associate, Chemistry Division, Bioscience Division, and Computer and Computational Sciences Division, Los Alamos National Laboratory. Postdoctoral advisor: Jill Trehwella
2001-present	Technical Staff Member, Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory
2001-present	Affiliate, Bioscience Division
2005-present	Team Leader, Computational Biology and Bioinformatics
2007-present	Affiliate, Center for Nonlinear Studies
2009-present	Executive Committee Member, Center for Nonlinear Studies

### **Honors and Awards**

Keck Center for Computational Biology NSF Postdoctoral Fellowship (1996-1998); Robert A. Welch Foundation Postdoctoral Fellowship (1996-1999); Best poster presentation, Keck Center Annual Research Conference on Computational Biology (1997)

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### **Professional Activities**

Cultural exchange: Invited participant, 6<sup>th</sup> Annual Japanese-American Beckman Frontiers of Science Symposium (Japanese Society for the Advancement of Science, US National Academy of Sciences), Kanagawa, Japan (Dec 2003)

Meeting organization: First, Second, and Third q-bio Conference on Cellular Information Processing (Santa Fe, 2007-2009); First, Second, and Third q-bio Summer School on Cellular Information Processing (Los Alamos, 2007-2009); Theory, Simulations, and Computing Capability Workshop on Computational Systems Biology (LANL, Oct 2006)

Referee for over 20 journals and multiple national and international funding agencies.

Organizational review: Member of extramural review panel, Department of Biostatistics, Bioinformatics, and Epidemiology, Medical University of South Carolina (Sep 2008)

Professional society memberships: American Physical Society (1990-present); Biophysical Society (1992-present)

### **Invited Talks**

Department of Pharmacology, Bioinformatics course, 10/27/2009, University of Colorado, Denver, CO. Invited lecture: Protein Structure.

Department of Pharmacology, 10/26/2009, University of Colorado, Denver, CO. Invited talk: Ligand Binding, Protein Dynamics, and Function Prediction.

Regulation of Protein Phosphorylation: Energy Landscapes, Allostery, and Dynamic Regulation, 12/5-12/7/2008, UC-San Diego, La Jolla, CA. Invited talk: Modulation of the kinase ensemble by second messengers.

Second q-bio Conference on Cellular Information Processing, 8/6-8/9/2008, Santa Fe, NM. Invited talk: Diverse mechanisms of transcriptional activation in the *Escherichia coli* *marA/soxS/rob* regulon.

Characterizing Landscapes: From Biomolecules to Cellular Networks, 7/7/-7/11/2008, Telluride Science Research Center, Telluride, CA. Invited talk: Ligand-Induced Perturbation of Protein Energy Landscapes.

Workshop on Principles of Biological Computation, 18-21 May 2008, Santa Fe Institute, Santa Fe, NM. Invited talk: Signal transduction using real proteins.

Department of Biochemistry, 4/29/2008, University of Otago, Dunedin, New Zealand. Invited talk: Protein Dynamics and Ligand Binding: Computational Insights into Allostery.

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SIMBIOS NIH Center for Biomedical Computing, 4/16/2008, Stanford University, Stanford, CA. Invited talk: Computational Insights into Allostery, with Bioinformatics Applications.

Department of Computational Biology, 11/7/07, University of Pittsburgh Medical Center, Pittsburgh, PA. Invited talk: Computational studies of protein function using dynamics perturbation analysis.

Bioinformatics Research Center, 9/7/07, University of North Carolina, Charlotte, NC. Invited talk: Protein interactions and energy landscapes.

Workshop on Small-Angle X-ray Scattering in Biological Sciences, 5/31/07-6/1/07, Colorado State University, Fort Collins, CO. Invited talk: Large-scale shape changes associated with activation of cGMP-dependent protein kinase.

Department of Microbiology, University of Otago, Dunedin, New Zealand, 12/15/2006. Invited colloquium: Computational modeling of gene regulation in *Escherichia coli*.

Second International Conference of the Biocomputing and Physics of Complex Systems Research Institute (BIFI), University of Zaragoza, Zaragoza, Spain. 8-11 February 2006. Invited talk: Principles of Biochemical Regulation. Session chair.

13th Annual International Meeting on Microbial Genomics, University of Wisconsin, Madison, WI. 11-15 September 2005. Invited talk: Computational Models of Biochemical Regulation.

The third annual retreat of the Computation and Informatics in Biology and Medicine Training Program, University of Wisconsin, Madison, WI. 15 October 2004. Invited talk: Design principles of genetic regulatory networks.

International Conference on Molecular Systems Biology 2004, 8/21/04-8/25/04, Tahoe City, CA. Invited talk: Design principles of genetic regulatory networks.

Institute for Pure and applied Mathematics, 4/1/04, UCLA, Los Angeles. Invited colloquium: Structure and function of genetic regulatory circuits in *Escherichia coli*.

MIPNETS workshop on Proteins and Signals, 6/25/2003, Liverpool, UK. Invited talk: Mechanisms of Biochemical Regulation. Session chair.

University of Otago, 5/2/2003, Dunedin, New Zealand. Invited talk: Mechanisms of biochemical regulation.

American Physical Society meeting, 3/2/2003, Austin TX. Invited tutorial: Transcriptional Regulatory Networks: Data, Analysis and Modeling

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LANL workshop on enabling concepts in systems biology, 9/19/2002, Santa Fe, NM. Invited talk: Integrating systems and structural biology: structural mechanisms in cGMP binding and activation of cGMP-dependent protein kinase

American Chemical Society Rocky Mountain Regional Meeting, 10/14/2002, Albuquerque, NM. Invited talk: Mechanisms associated with cGMP binding and activation of cGMP-dependent protein kinase

Instituto Gulbenkian de Ciencia, 3/11-3/15/2002, Oeiras, Portugal. Institute-sponsored visit; bioinformatics lectures on microarray methods.

APS User Meeting, 10/9/2001, Argonne National Laboratory, Argonne, IL. Invited talk: Diffuse Scattering: Methods for Molecular Structure and Dynamics

LANL/UCSD Workshop, 9/8/2001-9/9/2001, San Diego, CA. Invited talk: Diffuse Scattering and Database Methods

National Center for Genome Resources, March 2001, Santa Fe, NM. Invited seminar: Singular value decomposition analysis of microarray data

Gordon Research Conference on Diffraction Methods in Molecular Biology, Summer 2000, Andover, NH. Invited talk: Harnessing the potential of a structure database

Los Alamos National Laboratory, February 1999, Los Alamos, NM. Invited talk: Refinement of X-ray structures using a database of pairwise interatomic distance probabilities

School of Biological Sciences, December 1998, Auckland University, Auckland, New Zealand. Invited talk: Dynamics in Calmodulin

Department of Chemistry, December 1998, Massey University, Palmerston North, New Zealand. Invited talk: Dynamics in Calmodulin

Department of Biochemistry, December 1998, Otago University, Dunedin, New Zealand. Invited talk: Dynamics in Calmodulin

Gordon Research Conference on Diffraction Methods in Molecular Biology, Summer 1998, Andover, NH. Invited talk: Making sense of diffuse scattering and making use of all the X-rays

Parke-Davis Pharmaceuticals, Spring 1998, Ann Arbor, MI. Two invited talks: Dynamics in calmodulin crystals; Refinement of X-ray structures using a database of pairwise interatomic distance probabilities

Biophysical Society Meeting, Winter 1998, Kansas City, MO. Invited talk: Refinement of X-ray structures using a database of pairwise atomic distance probabilities

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Department of Molecular and Cellular Biology, Fall 1997, Brown University, Providence, RI.  
Invited talk: Dynamics in calmodulin crystals

International Union of Crystallography Meeting, August 1996, Seattle, WA. Invited talk on  
dissertation research

CHESS Journal Club, May 1996, Cornell University, Ithaca, NY. Invited talk on dissertation  
research

Keck Center for Computational Biology Colloquium, September 1995, Rice University,  
Houston, TX. Invited talk on dissertation research

DCRT Structural Biology Division, 1994, National Institutes of Health, Bethesda, MD. Invited  
talk on dissertation research

### Software and Databases

1. LUNUS – Software for diffuse X-ray scattering from protein crystals (<http://lunus.sf.net>)
2. SOESA – Structure Optimization and Evaluation using Separations of Atom  
(<http://public.lanl.gov/mewall/soesa.tar> )
3. SVDMAN – Singular Value Decomposition Microarray Aalysis  
(<http://public.lanl.gov/svdman>)
4. EcoTFs – *E. coli* Transcription Factors and Signals Database (with William S. Hlavacek,  
<http://ecotfs.lanl.gov>)

### Publications in Peer-Reviewed Journals

1. S.M. Gruner, S.L. Barna, M.E. Wall, M.W. Tate, E.F. Eikenberry. 1993. Characterization  
of polycrystalline phosphors for area X-ray detectors. Proceedings of the SPIE - The  
International Society for Optical Engineering 2009:98-108
2. M.W. Tate, E.F. Eikenberry, S.L. Barna, M.E. Wall, J.L. Lowrance, S.M. Gruner. A  
large-format high-resolution area X-ray detector based on a fiber-optically bonded  
charge-coupled device (CCD). 1995. Journal of Applied Crystallography 28:196-205
3. R.L. Walter, D.J. Thiel, S.L. Barna, M.W. Tate, M.E. Wall, E.F. Eikenberry, S.M. Gruner  
and S.E. Ealick. 1995. High-resolution macromolecular structure determination using  
CCD detectors and synchrotron radiation. Structure 3:835
4. M.E. Wall, S.E. Ealick and S.M. Gruner. 1997. Three-dimensional diffuse X-ray  
scattering from crystals of *Staphylococcal nuclease*. Proc Natl Acad Sci USA 94:6180-84
5. M.E. Wall, J.B. Clarage and G.N. Phillips, Jr. 1997. Motions of calmodulin characterized  
using both Bragg and diffuse X-ray scattering. Structure 5:1599-1612
6. M.E. Wall, S. Subramaniam and G.N. Phillips, Jr. 1999. Protein structure determination  
using a database of interatomic distance probabilities. Protein Sci 8:2720-27.

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7. C.S. Tung, M.E. Wall, S.C. Gallagher and J. Trehwella. 2000. A model of troponin-I in complex with troponin-C using hybrid experimental data: the inhibitory region is a  $\beta$ -hairpin. *Protein Sci* 7:1312-26
8. M.E. Wall, P.A. Dyck and T.S. Brettin. 2001. SVDMAN – singular value decomposition analysis of microarray data. *Bioinformatics* 6:566-568
9. M.E. Wall, S.H. Francis, J.D. Corbin, K. Grimes, R. Richie-Jannetta, J. Kotera, B.A. Macdonald, R.R. Gibson and J. Trehwella. 2003. Mechanisms associated with cGMP binding and activation of cGMP-dependent protein kinase. *Proc Natl Acad Sci USA* 100:2380-2385.
10. M.E. Wall, W.S. Hlavacek and M.A. Savageau. 2003. Design principles for regulator gene expression in a repressible gene circuit. *J Mol Biol* 332:861-876.
11. D. Ming and M.E. Wall. 2005. Quantifying allosteric effects in proteins. *Proteins* 59:697-707.
12. M.E. Wall, M.J. Dunlop and W.S. Hlavacek. 2005. Multiple functions of a feed-forward-loop gene circuit. *J Mol Biol* 349:501-514
13. D. Ming and M.E. Wall. 2005. Allostery in a coarse-grained model of protein dynamics. *Phys Rev Lett* 95:198301
14. D. Ming and M.E. Wall. 2006. Interactions in native binding sites cause a large change in protein dynamics. *J Mol Biol* 358:213-223
15. D. Ming, M.E. Wall, and K.Y. Sanbonmatsu. 2007. Domain motions of Argonaute, the catalytic engine of RNA interference. *BMC Bioinformatics* 8:470 (“Highly accessed” designation).
16. D. Ming, M. Anghel, and M.E. Wall. 2008. Hidden structure in protein energy landscapes. *Phys Rev E* 77:021902.
17. D. Ming, J.D. Cohn, and M.E. Wall. 2008. Fast dynamics perturbation analysis for prediction of protein functional sites. *BMC Struct Biol* 8:5.
18. R. G. Martin, E. S. Bartlett, J. L. Rosner, M. E. Wall. 2008. Activation of the *Escherichia coli* *marA/soxS/rob* regulon in response to transcriptional activator concentration. *J Mol Biol* 380:278-284.
19. D.W. Dreisigmeyer, J. Stajic, I. Nemenman, W.S. Hlavacek, M.E. Wall. 2008. Determinants of bistability in induction of the *Escherichia coli* *lac* operon. *IET Syst Biol* 5:293-303
20. M. E. Wall, D. A. Markowitz, J. L. Rosner, R. G. Martin. 2009. Model of transcriptional activation by MarA in *Escherichia coli*. *PLoS Computational Biology* 5:e1000614.

### Peer-Reviewed Conference Proceedings

21. M.J. Dunlop and M.E. Wall. 2005. Robustness in gene circuits: clustering of functional responses. *Proceedings of the 24th American Control Conference* 6:4411-4416
22. M.E. Wall. Ligand binding, protein fluctuations, and allosteric free energy. 2006. *AIP Conference Proceedings* 851:16-33
23. I. Nemenman, G.S. Escola, W.S. Hlavacek, P.J. Unkefer, C.J. Unkefer, M.E. Wall. 2007. Reconstruction of metabolic networks from high-throughput metabolite profiling data: *in silico* analysis of red blood cell metabolism. *Ann NY Acad Sci* 1115:102-115

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### **Review Articles**

24. M.E. Wall, S.C. Gallagher and J. Trewhella. 2000. Large-scale shape changes in proteins and macromolecular complexes. *Ann Rev Phys Chem* 51:355-80
25. M.E. Wall, W.S. Hlavacek and M.A. Savageau. 2004. Design of gene circuits: lessons from bacteria. *Nat Rev Genet* 5:34-42.

### **Book Chapters**

26. M.E. Wall, A. Rechtsteiner, L.M. Rocha. 2003. Singular Value Decomposition and Principal Component Analysis. In *A Practical Approach to Microarray Data Analysis*. D.P. Berrar, W. Dubitzky, M. Granzow, eds. pp. 91-109, Kluwer:Norwell, MA.
27. M.E. Wall. 2009. Methods and software for diffuse X-ray scattering from protein crystals. *Meths Mol Biol* 544:269-279.

### **Editorials**

28. I. Nemenman, W.S. Hlavacek, J.S. Edwards, J.R. Faeder, Y. Jiang, M.E. Wall. 2008. Selected papers from the First q-bio Conference on Cellular Information Processing. *IET Syst Biol* 5:203-205
29. I. Nemenman, W. S. Hlavacek, Y. Jiang, M. E. Wall. 2009. Editorial: Selected papers from the Second q-bio Conference on Cellular Information Processing. *IET Syst Biol* 3:297.

### **News Features**

30. J.S. Edwards, J.R. Faeder, W.S. Hlavacek, Y. Jiang, I. Nemenman, and M.E. Wall. 2007. q-bio 2007: A Watershed Moment in Modern Biology. *Mol Syst Biol* 3:148